Theory and Practice of Molecular Electronic Structure

Course number: 545 (4 units)

FACULTY:

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OBJECTIVE:

To provide working knowledge and hands-on experience in current quantum chemical methods for chemists, who would like to employ these techniques in their own research.

COURSE DESCRIPTION:

The course is dedicated to providing a solid and deep understanding of the fundamentals and machinery of electronic structure theory and main concepts of quantum chemistry. Homework includes analytical problems requiring advanced analytical skills as well as computational assignments designed for hands-on experience with current quantum chemical methods and packaged programs. The course includes a midterm exam and an individualized computational mini research project. The project will be summarized in a term paper. The paper should contain introductory notes describing chemical problem and outlining the computational part, as well as a brief review of the literature. The bulk of the paper is presentation of results of the computations, followed by a discussion and a critical analysis. The project will be evaluated by the following criteria: (i) relevance the proposed computational experiment to the specific chemical problem; (ii) the completeness of the performed computations and the quality of presentation; (iii) correctness of the reported results; (iv) quality of analyses of the results.

PREREQUISITES:

Graduate level Quantum Mechanics and Mathematical Methods. Basic familiarity with Unix operational system is also required.

REQUIRED TEXTBOOK:

"Modern Quantum Chemistry. Introduction to Advanced Electronic Structure Theory" by A. Szabo and N.S. Ostlund. Additional materials will be supplied. Reading assignments will follow the course textbook and the handouts when appropriate.

CREDIT DISTRIBUTION:

- Homework 30%.
- Unannounced quizzes: 25%
- Midterm examination: 30%

- Final mini-project and presentation: 15%

TIME AND PLACE:

Lecture: SSC 604, 10:30-11:50 TTh.
Discussion hour: SSC 604 5:00-6:00 F (if needed).
Some sessions may take place on zoom.

COURSE WEBPAGE:

General: http://iopenshell.usc.edu/chem545.html
Full content: On blackboard.

SYLLABUS:

- Preliminaries: central approximations and important concepts in modeling.
  - Non-relativistic Schrödinger quantum mechanics;
  - Adiabatic approximation;
  - Attributes of an exact and approximate wave functions and energies: spatial symmetry, spin, variational properties, and size-consistency;
  - Concepts of scaling and predictiveness;
  - Exponential scaling of the exact solution.
- Self-Consistent Field Method (mean-filed model). Derivation of Hartree-Fock equations and MO-LCAO method.
- One-electron basis sets.
- Performance and limitations of Hartree-Fock model. Restricted and unrestricted HF and the symmetry dilemma.
- The correlation problem and methods to describe correlation.
  - Dynamical and non-dynamical correlation and their chemical consequences;
  - Perturbation theory, configuration interaction, coupled-cluster methods;
  - Potential energy surfaces by multi-reference and single reference techniques;
  - Achieving chemical accuracy.
- Density Functional methods.
- Chemical insight from electronic structure calculations calculations; analysis of wave functions and charge distributions.
- Electronically excited states; radiative and radiationless processes; molecular decomposition.

TENTATIVE SCHEDULE:

See course's website for previous years coverage.